COMPONENTS:	EVALUATOR:
(1) Naphthalene; C <sub>10</sub> H <sub>8</sub> ; [91-20-3] (2) Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	March 1986.

### CRITICAL EVALUATION:

Quantitative data for the solubility of naphthalene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Studies of the Solubility of Naphthalene (1) in Water (2)

Reference	T/K	Method
Hilpert (ref 1)	273,298	gravimetric
Mitchell (ref 2)	288,298	interferometric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Bohon and Claussen (ref 5)	273-316	spectrophotometric
Wauchope and Getzen (ref 6)	273-348	spectrophotometric
Eganhouse and Calder (ref 7)	298	GLC
Mackay and Shiu (ref 8)	298	spectrofluorometric
Schwarz and Wasik (ref 9)	285-298	spectrophotometric
Schwarz (ref 10)	282-305	spectrophotometric
May et al. (ref 11)	298	HPLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data appear to have been published on the solubility of water in naphthalene.

Despite the low solubility of naphthalene in water the published data are in excellent agreement. With the exception of the 298K data of Mitchell (ref 2) and Klevens (ref 4) which differ markedly from other studies, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

TABLE 2: Recommended (R) and Tentative Values of the Solubility of Naphthalene (1) in Water (2)

1			
T/K	Solubili	ty values	_
	Reported values $^a$	"Best" values	( ± σ <sub>n</sub> ) <sup>b</sup>
	10 <sup>3</sup> g(1)/100g sln	10 <sup>3</sup> g(1)/100g sln	10 <sup>6</sup> x <sub>1</sub>
273	1.9 (ref 1), 1.37 (ref 5), 1.37 (ref 6)	1.5 ± 0.2	2.1
283	1.94 (ref 5), 2.0* (ref 6), 1.87* (ref 10)	1.9 ± 0.1 (R)	2.7 (R)
		(Table 2 continued n	ext page)

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### **EVALUATOR:**

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March, 1986.

CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility	values	· · · · · · · · · · · · · · · · · · ·
-,	Reported values <sup>a</sup> $10^3 g(1)/100g sln$	"Best" values	
293	2.86* (ref 5), 2.8* (ref 6), 2.62* (ref 10)	2.8 ± 0.1 (R)	3.9 (R)
298	3.0 (ref 1), 3.15 (ref 3), 3.44 (ref 5), 3.12 (ref 6), 3.13 (ref 7), 3.17 (ref 8), 3.00 (ref 9), 3.03 (ref 10), 3.17 (ref 11)	3.1 ± 0.1 (R)	3.9 (R)
303	4.3* (ref 5), 3.7* (ref 6), 3.48* (ref 10)	3.8 ± 0.3	5.3
313	6.6* (ref 5), 5.5* (ref 6)	6.1 ± 0.6	8.6
323	8.24* (ref 6)	8.2	12
333	13.0* (ref 6)	13	18
343	20.0* (ref 6)	20	28
348	25.8 (ref 6)	26	37

lpha Values marked with an asterisk (\*) were obtained by the Evaluator by graphical interpolation. b Obtained by averaging where appropriate;  $\sigma_n$  has no statistical signifi-

cance.

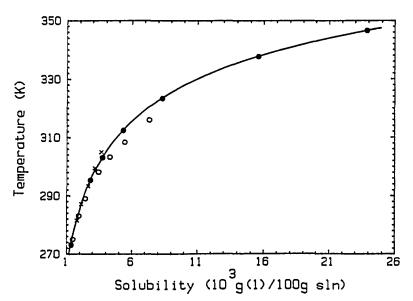


FIGURE 1. Solubility of naphthalene in water, selected data: ret 5 (0); ref 6 (•); ref 10 (x). Solid curve fitted through "Best" values (Table 2).

(continued next page)

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

March, 1986.

CRITICAL EVALUATION: (continued)

### REFERENCES

- 1. Hilpert, S. Angew. Chem. 1916, 29, 57-9.
- 2. Mitchell, S. J. Chem. Soc. 1926, 129, 1333-6.
- 3. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-77.
- 4. Klevens, H.B. J. Phys. Chem. 1950, 54, 283.
- 5. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. 1951, 73, 1571-8.
- 6. Wauchope, R.D.; Getzen, F.W. J. Chem. Eng. Data 1972, 17, 38-41.
- 7. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, 40, 555-61.
- 8. Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data 1977, 22, 399-402.
- 9. Schwarz, F.P.; Wasik, S.P. J. Chem. Eng. Data 1977, 22, 270-3.
- 10. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- 11. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000.

### ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

### 239 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3] Hilpert, S. (2) Water; H<sub>2</sub>O; [7732-18-5] Angew. Chem. 1916, 29, 57-9. VARIABLES: PREPARED BY: Temperature: 0 and 25°C A. Maczynski and A. Szafranski EXPERIMENTAL VALUES: Solubility of naphthalene in water

t/°C	10 <sup>3</sup> g(1)/100 g sln	$\frac{10^6 x_1}{}$	
0	1.9	2.7	
25	3.0	4.2	

### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A sample of (1) was shaken with 1000 g(2) until saturation and then filtered. The filtrate was steam distilled to drive away (1) which was collected and presumably weighed.	(1) not specified. (2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Mitchell, S.

J. Chem. Soc. London 1926, 1332-6.

### VARIABLES:

Temperature: 15 and 25°C

### PREPARED BY:

A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

### Solubility of naphthalene in water

t/°C	g(1) L <sup>-1</sup> (2)	g(1)/100 g sln (compiler)	$\frac{10^6 x_1}{}$ (compiler)
15	0.022	0.0022	3.1
25	0.040	0.0040	5.6

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

For this study an interferometer of the type described in ref (1) was constructed.

### SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

### ESTIMATED ERROR:

not specified.

### REFERENCES:

1. Jamin Ann. Chim. Phys. 1958, 52, 171.

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1949, 71, 3644-77.

### VARIABLES:

One temperature: 25°C

### PREPARED BY:

A. Maczynski and Z. Maczynska

### **EXPERIMENTAL VALUES:**

The solubility of naphthalene in water at 25°C was reported to be 0.00315 g(1)/100 g sln.

The corresponding mole fraction,  $x_1$ , value calculated by compiler is  $4.42 \times 10^{-6}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

### SOURCE AND PURITY OF MATERIALS:

- (1) Eastman Kodak Co., best grade; recrystallized from ethanol; mp. 80.5°C.
- (2) not specified.

### ESTIMATED ERROR:

not specified.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; C <sub>10</sub> H <sub>8</sub> ; [91-20-3] (2) Water; H <sub>2</sub> O; [7732-18-5]	Klevens, H.B.  J. Phys. Chem. <u>1950</u> , 54, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 0.0125 g(1)  $L^{-1}$  sln and 9.75 x  $10^{-5}$  mol(1)  $L^{-1}$  sln. Assuming that 1.00 L sln = 1.00 kg sln, the corresponding values calculated by the compiler are 0.00125 g(1)/100 g sln and mole fraction,  $x_1$ , = 1.76 x  $10^{-6}$ .

# METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra. ESTIMATED ERROR: not specified. ESTIMATED ERROR: not specified. REFERENCES:

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Bohon, R.L.; Claussen, W.F.

J. Am. Chem. Soc. 1951, 73, 1571-8.

### VARIABLES:

Temperature:

0-42.8°C

PREPARED BY:

G.T. Hefter

### EXPERIMENTAL VALUES:

Solubility of naphthalene in wa	ter	Wa	in	ene	ithal	napl	of	itv	Solubil
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t/°C	10 <sup>3</sup> g(1)/100g sln <sup>a</sup> (compiler)	$10^{6}x_{1}$
	1 27	1 02
0.0	1.37	1.92
0.4	1.37	1.92
0.5	1.38	1.94
0.9	1.46	2.05
1.9	1.50	2.11
9.4	1.96	2.75
10.0	1.94	2.72
14.9	2.34	3.29
15.9	2.46	3.45
19.3	2.80 3.44b	3.93 4.83 <i>b</i>
25.0	3.44 <sup>D</sup>	4.83 <sup>D</sup>
25.6	3.58	5.03
30.1	4.30	6.04
30.2	4.39	6.16
35.2	5.45	7.65
36.0	5.48	7.69
42.8	7.35	10.3

a Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

 $^{b}$  Given in the paper as 0.0344g(1)/L sln.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

### SOURCE AND PURITY OF MATERIALS:

- (1) Allied Chemical & Dye Corp., purified by vacuum distillation.
- (2) Air-free conductivity water, no other details given.

ESTIMATED ERROR:
Temp. ± 0.02°C
Soly. ± 0.5% relative

### COMPONENTS: (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3] Wauchope, R.D.; Getzen, F.W. (2) Water; H<sub>2</sub>O; [7732-18-5] J. Chem. Eng. Data 1972, 17, 38-41. VARIABLES: Temperature: 0-75°C PREPARED BY: A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of naphthalene in water

	mg(1)/kg	(2)	•	6
t/°C	experiment	smoothed with (std dev)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
	experiment	(800 007)	(COMPLECT)	<u> </u>
0.0		13.7(0.2)	0.00137	1.93
22.2	28.8, 29.1, 28.8	28.3	0.00283	3.98
24.5	30.8(2), 30.1(2),	30.7 30.7	0.00307	4.31
25.0		31.2(0.2)	0.00312	4.38
29.9	38.1, 38.2, 38.3	37.3	0.00373	5.24
30.3	38.1, 37.6, 37.6	37.8	0.00378	5.31
34.5	44.6, 43.8	44.3	0.00443	6.23
39.2	52.6, 52.8	53.3	0.00533	7.49
40.1	54.8	55.0	0.00550	7.73
44.7	66.0, 65.5, 65.3	66.2	0.00662	9.30
50.0	•	82.4(0.4)	0.00824	11.58
50.2	78.6	83.1	0.00831	11.68
55.6	106	105	0.0105	14.8
64.5	166, 151, 157	156	0.0156	21.9
73.4	240, 247, 244	239	0.0239	33.6
75.0		258(3)	0.0258	36.3

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared

Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

### SOURCE AND PURITY OF MATERIALS:

- (1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.
- (2) distilled and deionized.

### ESTIMATED ERROR:

temp. ± 0.5°C

soly. see experimental values above

### ORIGINAL MEASUREMENTS: COMPONENTS: (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3] Eganhouse, R.P.; Calder, J.A. (2) Water; H<sub>2</sub>O; [7732-18-5] Geochim. Cosmochim. Acta 1976, 40, 555-61. VARIABLES: PREPARED BY: One temperature: 25°C A. Maczynski

### EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 31.3 mg(1)/kg(2) and 2.43 x  $10^{-4}$  mol(1) dm<sup>-3</sup>(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 3.13 x  $10^{-3}$  g(1)/100 g sln and  $\frac{1}{4}$ .40 x  $10^{-6}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

### SOURCE AND PURITY OF MATERIALS:

- (1) source not specified; analytical grade; used as received; no impurities by glc.
- (2) double distilled; free of trace organics.

### ESTIMATED ERROR:

temp. ± 0.5°C

 $soly. \pm 0.4 mg(1)/kg(2)$ 

(from eight determinations)

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, 22, 399-402.

### **VARIABLES:**

One temperature: 25°C

### PREPARED BY:

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 31.7 mg(1) dm<sup>-3</sup> sln and  $x_1 = 4.46 \times 10^{-6}$ .

The corresponding mass percent calculated by the compiler is 0.00317 g(1)/100 g sln.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

### SOURCE AND PURITY OF MATERIALS:

- (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
- (2) doubly distilled.

### ESTIMATED ERROR:

soly.  $\pm$  0.26 mg(1) dm<sup>-3</sup> sln (maximum deviation from several determinations).

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, 22, 273-7.

### VARIABLES:

PREPARED BY:

Temperature: 8.4-31.8°C

A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of naphthalene in water

t/°C	10 <sup>4</sup> mol(1) L <sup>-1</sup>	10 <sup>3</sup> g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
8.4	1.40 ± 0.02	1.79	2.52
11.1	1.49 ± 0.03	1.91	2.68
14.0	1.66 ± 0.05	2.13	2.99
17.5	1.88 ± 0.03	2.41	3.39
20.2	2.07 ± 0.02	2.65	3.73
23.2	2.22 ± 0.03	2.85	4.00
25.0	2.36 ± 0.02	3.03	4.25
26.3	2.48 ± 0.02	3.18	4.47
29.2	2.68 ± 0.02	3.44	4.83
31.8	2.83 ± 0.02	3.63	5.10

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

### SOURCE AND PURITY OF MATERIALS:

- (1) source not specified; better than 99.9 mole\*, by glc; used as received.
- (2) distilled over KMnO<sub>4</sub> and NaOH and passed through a Sephadex column.

### ESTIMATED ERROR:

temp. ± 0.1°C soly. see above

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Schwarz, F.P.; Wasik, S.P.

J. Chem. Eng. Data 1977, 22, 270-3.

### VARIABLES:

Temperature: 12-25°C

### PREPARED BY:

A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of naphthalene in water

t/°C	10 <sup>4</sup> mol(1) L <sup>-1</sup>	10 <sup>3</sup> g(1)/100 g sln (compiler)	10 <sup>6</sup> x <sub>1</sub> (compiler)
12	1.57	2.01	2.83
18	1.90	2.43	3.42
25	2.34	3.00	4.21

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.

### SOURCE AND PURITY OF MATERIALS:

- (1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%.
- (2) distilled from KMnO<sub>4</sub> and passed through a Sephadex column.

### ESTIMATED ERROR:

temp.  $\pm 0.1^{\circ}C$ soly.  $\pm 2 \times 10^{-6}$  mol(1) dm<sup>-3</sup>

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000.

### VARIABLES:

One temperature: 25°C

### PREPARED BY:

A. Maczynski

### EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 31.69 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , values calculated by compiler are 0.003169 g(1)/100 g sln and 4.425 x  $10^{-6}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

### SOURCE AND PURITY OF MATERIALS:

- (1) commercial product; less than 3% impurities.
- (2) distilled over KMnO<sub>4</sub> and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

### ESTIMATED ERROR:

temp. ± 0.05°C

soly. ± 0.23 mg(1)/100 kg(2) (standard deviation)

### REFERENCES:

 May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. J. Chromatogr. Sci. 1975, 13, 535.

- (1) Naphthalene;  $C_{10}H_{8}$ ; [91-20-3]
- (2) Seawater

**EVALUATOR:** 

D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA

December 1982

### CRITICAL EVALUATION:

The solubility of naphthalene (1) in seawater (2) has been reported in six works:

Authors		Method	T/K	Salinity g salts/kg sln	10 <sup>3</sup> g(1)/100 g sln
Paul (ref 1)	uv	spectral	298	30.59	2.53
Gordon and Thorne (ref 2)	uv	spectral	298	35.0	2.36
Gordon and Thorne (ref 3)	uv	spectral	298	31.7	2.47
Eganhouse and Calder (ref 4)		GLC	298	35	2.20
Schwarz (ref 5)	uv	spectral	298	30	2.17
May et al. (ref 6)		HPLC	298	35.0	2.29

At 298 K and a salinity of 35 g salts/kg sln the data of Gordon and Thorne (ref 2), Eganhouse and Calder, and May et al. are in good agreement. Therefore the mean value, 2.29 x 10<sup>-3</sup>, is adopted as the recommended value at this temperature and salinity. Since the value of Schwarz is lower than would be expected with decreasing salinity, it is considered doubtful. At 298 K and a salinity of 31 g salts/kg sln the data of Paul and of Gordon and Thorne (ref 3) are in fair agreement. Therefore their mean is adopted as a tentative value. Gordon and Thorne (ref 2) and May et al. report data for a range of salinities using the Setschenow equation. Schwarz reports data over the temperature range 281 to 303 K. However, since this data at 298 K appears low, the usefulness of this work is diminished.

### SOLUBILITY OF NAPHTHALENE (1) IN SEAWATER (2) RECOMMENDED(r) AND TENTATIVE(t) VALUES

T/K	g salts/kg sln	$10^3 g(1)/100 g sln$	
298	35 (r)	2.29	
298	31 (t)	2.5	

- Paul, M.A. J. Amer. Chem. Soc. 1952, 74, 5274-7.
- 2. Gordon, J.E.; Thorne, R.L. J. Phys. Chem. 1967, 71, 4390-9.
- 3. Gordon, J.E.; Thorne, R.L. Geochim. Cosmochim. Acta 1967, 31, 2433-43.
- 4. Eganhouse, R.P.; Calder, J.A. Geochim. Cosmochim. Acta 1976, 40,
- 5. Schwarz, F.P. J. Chem. Eng. Data 1977, 22, 273-7.
- 6. May, W.E.; Wasik, S.P.; Freeman, D.H. Anal. Chem. 1978, 50, 997-1000.

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Sodium chloride; NaCl; [7732-14-5]
- (3) Water; H<sub>2</sub>O; [7647-18-5]

### ORIGINAL MEASUREMENTS:

Paul, M.A.

J. Am. Chem. Soc. 1952, 74, 5274-7.

### VARIABLES:

One temperature: 25°C

Salinity: 13-64 g(3)/kg sln

### PREPARED BY:

M. Kleinschmidt and W. Shiu

### EXPERIMENTAL VALUES:

Solubility of Naphthalene in Aqueous Sodium Chloride

g(2)/kg sln*	10 <sup>4</sup> g-mol(1)/L <sup>-1</sup>	10 <sup>3</sup> Mass %*	10 <sup>6</sup> × <sub>1</sub> *
12.40	2.37	3.01	4.27
25.31	2.00	2.52	3.61
30.59	2.02	2.53	3.64
43.70	1.68	2.09	3.02
61.63	1.38	1.69	2.48
	12.40 25.31 30.59 43.70	12.40 2.37 25.31 2.00 30.59 2.02 43.70 1.68	12.40 2.37 3.01 25.31 2.00 2.52 30.59 2.02 2.53 43.70 1.68 2.09

<sup>\*</sup>Calculated by compilers using density and other physical data for NaCl solutions from ref 1.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Equilibration flask: 50-mL glass-stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken vigorously while cooling until excess hydrocarbon had recrystallized. The flask was then placed into a water bath thermostatically controlled at 25.00 ± 0.05°C for at least 48 hr, and shaken occasionally during that time. Samples were withdrawn with a 10-ml transfer pipet, diluted appropriately and analyzed using a spectrophotometer in the ultra-violet region of the spectrum.

### SOURCE AND PURITY OF MATERIALS:

- (1) recrystallized from menthanol
- (2) reagent grade, dried at 120°C before weighing
- (3) redistilled

Sources not specified.

### ESTIMATED ERROR:

temp. ± 0.05°C

soly. ± 1 %

### REFERENCES:

1. Weast, R.C.; CRC Handbook of Chemistry and Physics, 59th Edition; CRC Press 1978, pp D299-D300.

## COMPONENTS: (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3] Gordon, J.E.; Thorne, R.L. (2) Sodium chloride; NaCl; J. Phys. Chem. 1967, 71, 4390-9. [7647-14-5] (3) Water; H<sub>2</sub>O; [7732-18-5] VARIABLES: PREPARED BY: One temperature: 24.91°C M. Kleinschmidt and D. Shaw Salinity: 0-108 g(2)/kg sln

EXPERIMENTAL VALUES:

The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$log(S_O/S) = K_SC_S$$

where,  $S_{\rm O}$  is the solubility of naphthalene in water (mol/L) S is the solubility of naphthalene in solution (mol/L)  $K_{\rm S}$  is the Setschenow constant (L/mol)  $C_{\rm S}$  is the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of  $C_{\rm S}$  0-2 mol/L, log  $S_{\rm O}$  = -3.590  $\pm$  0.004 (95% confidence limit) and  $K_{\rm S}$  = 0.220  $\pm$  0.0041 (95% confidence limit).

The corresponding mass percent and mole fraction,  $x_1$  at salinity = 35 g(2)/kg sln calculated by the compilers are 2.36 x  $10^{-3}$  g(1)/100 g sln and 3.48 x  $10^{-6}$  assuming a solution density of 1.025 kg/L.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Saturated solutions were prepared by equilibrating excess (1) in salt water in sealed ampols for 24 hrs. After filtration the absorbance was measured with a UV spectrophotometer at three wavelengths.

### SOURCE AND PURITY OF MATERIALS:

- (1) recrystallized four times and sublimed or zone refined, 99.99+% pure,
- (2) analytical reagent grade,
- (3) distilled from potassium permanganate and redistilled from all glass still.

### ESTIMATED ERROR:

temp. ± 0.03°C soly. see above

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) natural seawater

### ORIGINAL MEASUREMENTS:

Gordon, J.E.; Thorne, R.L.

Geochim. Cosmochim. Acta, 1967, 31, 2433-43.

### VARIABLES:

Une temperature: 25°C

Salinity: 10-32 g/kg sln

### PREPARED BY:

W.Y. Shiu and D. Mackay

### EXPERIMENTAL VALUES:

Salinity <sup>b</sup> g/kg sln	Chlorosity (°/)	Treatment <sup>a</sup>	log S Observed	10 <sup>4</sup> s <sup>b</sup> g-mol(1)/ dm <sup>3</sup>	10 <sup>3</sup> mass ratio <sup>b</sup> g(1)/100 g sln	10 <sup>6</sup> mole, fraction X 1
31.8	17.96	MF	-3.715	1.93	2.47	3.47
			-3.717	1.92	2.46	3.45
31.8	17.96	GFF	-3.713	1.94	2.48	3.49
			-3.712	1.94	2.49	3.49
31.9	18.00	CENT	-3.704	1.98	2.53	3.56
ı			-3.708	1.96	2.51	3.53
31.5	17.81	MF	-3.721	1.90	2.44	3.42
			-3.722	1.91	2.45	3.41
31.8	17.95	GFF	-3.719	1.90	2.43	3.44
			-3.722	1.91	2.45	3.41
31.7	17.72	MF	-3.715	1.93	2.47	3.45
			-3.716	1.92	2.465	3.46
31.5	17.80	GFF	-3.719	1.91	2.45	3.41
			-3.720	1.905	2.44	3.43
9.8	5.45	MF	-3.630	2.344	3.005	4.22
			-3.630	2.344	3.005	4.22
					(continued	)

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Detail given in reference (1). Saturated solutions were prepared by equilibrating excess naphthalene and salt solution in an ampoule with shaking for 24 hours. The filtered saturated solution was analyzed by a UV Spectrophotometer.

### SOURCE AND PURITY OF MATERIALS:

Naphthalene: 99.99 + % from James Hinton, Valparaiso,

Florida

Salts: Analytical reagent grade from Mallinckrodt

Natural Seawater: collected at West Falmouth, Buzzards Bay, Quicks Hole and Mashapaquit Creek,

Massachusetts

### ESTIMATED ERROR:

Solubility ± 3% (Authors)

Temperature ± 0.03°C (Authors)

### REFERENCES:

Gordon, J.E.; Thorne, R.L. J. Phys. Chem. 1967, 71, 4390.

### ORIGINAL MEASUREMENTS:

(1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]

Gordon, J.E.; Thorne, R.L.

(2) natural seawater

Geochim. Cosmochim. Acta 1967, 31, 2433-43.

Experimental Values: (continued)

Salinity <sup>b</sup> g/kg sln	Chlorosity (°/)	Treatment <sup>a</sup>	log s Observed	10 <sup>4</sup> 5 <sup>b</sup> . g-mol(1)/ dm <sup>3</sup>	10 <sup>3</sup> mass ratio <sup>b</sup> g(1)/100 q sln	10 <sup>6</sup> molebfraction
9.8	5.45	GFF	-3.629 -3.632		3.01 2.99	4.23

 $^{a}\text{MF, membrane }(0.45\mu)$  filtered; GFF, glass fiber filtered; CENT, centrifuged

bValues calculated by compiler.

Temperature = 24.91°C

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub> [91-20-3]
- (2) Artificial seawater (ref 1)

### ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, 40 555-61.

### VARIABLES:

One temperature: 25.0°C Salinity: 35 g/kg sln

### PREPARED BY:

M. Kleinschmidt and W. Shiu

### EXPERIMENTAL VALUES:

The solubility of naphthalene in seawater is reported to be 22.0 mg/kg sln. The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compilers are 2.20 x  $10^{-3}$  g(1)/100 g sln and 3.18 x  $10^{-6}$ .

Graphical results for other salinities are also reported.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Equilibrium flask: 1 L Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated 12+ hr at 215 rpm on a New Brunswick gyrotary shaker; a 24 hr stationary equilibrium period followed. Hydrocarbons were extracted with doubly-distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard.

Analysis: gas chromatography

### SOURCE AND PURITY OF MATERIALS:

(1) analytical grade salts for artificial seawater solution, reagent grade.

water: doubly distilled

### ESTIMATED ERROR:

temperature: ± 0.5°C

soly: ± 0.293 (95% confidence interval).

### REFERENCES:

Lyman, J.; Fleming, R.H.;
 J. Mar. Res. <u>1940</u>, 3, 135.

### ORIGINAL MEASUREMENTS: COMPONENTS: Schwarz, F.P. (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3] (2) Sodium chloride; NaCl; J. Chem. Eng. Data 1977, 22, 273-7. [7647-14-5] (3) Water; H<sub>2</sub>O; [7732-18-5] VARIABLES . PREPARED BY: Temperature: 8.6-31.8°C W.Y. Shiu, D. Mackay Salinity: 30 g(2)/kg sln

### **EXPERIMENTAL VALUES:**

Solubility of naphthalene in 0.5 g-mol(2)/dm<sup>3</sup>

<u>t/°C</u>	$10^4 \text{ mol(1)/L sln}$
8.6	0.84
11.1	0.92
14.0	1.09
17.1	1.23
20.0	1.37
23.0	1.58
25.0	1.73
31.8	2.22

The corresponding mass percent and mole fraction  $x_1$ , at 25.0°C calculated by the compilers are  $2.17 \times 10^{-3}$  g(1)/100 g sln and  $3.13 \times 10^{-6}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility of naphthalene in NaCl Naphthalene: purity > 99 mole % solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated Ethanol: reagent grade solution was prepared by adding excess amount of naphthalene to an air-tight lxl cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and The Spectrofluorimeter em-315 nm. 315 nm. The Spectrofluorimeter employed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

### SOURCE AND PURITY OF MATERIALS:

Sodium chloride: reagent grade Water: distilled over a KMnO4 -NaOH solution and passed

through a Sephadex column.

### **ESTIMATED ERROR:**

Solubility ± 3.3% (author) Temperature ± 0.1°C (author)

- (1) Naphthalene; C<sub>10</sub>H<sub>8</sub>; [91-20-3]
- (2) Sodium Chloride; NaCl; [7647-14-5]
- (3) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman D.H.

Anal. Chem. 1978, 50, 997-1000.

### VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

### PREPARED BY:

W.Y. Shiu and D. Mackay

### EXPERIMENTAL VALUES:

The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$log(S_o/S) = K_sC_s$$

where;

 $S_0$  is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K is the Setschenow constant (L/mol)

C in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of  $C_{_{\rm S}}$  0-0.7 mol/L,

 $K_s = 0.213 \text{ with } S_0 = 31.69.$ 

The corresponding mass percent and mole fraction  $x_1$ , at salinity = 35 g(2)/kg sln calculated by the compilers are 2.29 x  $10^{-3}$  g(1)/100 g sln and 3.29 x  $10^{-6}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C<sub>18</sub> stationary phase, then a wateractetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

### SOURCE AND PURITY OF MATERIALS:

- (1) greater than 97% pure.
- (2) reagent grade.
- (3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

### ESTIMATED ERROR:

temp ± 0.05°C K<sub>s</sub> ± 0.001

 $S_0 \pm 0.23$